Supporting Information for

N-methylbenzoaza-18-crown-6-ether Derivatives as Efficient Alkali Metal Cations Sensors: the Dipole Moment and First Hyperpolarizability

Ying Gao, Shi-Ling Sun, Hong-Liang Xu, Liang Zhao and Zhong-Min Su**

Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University,

Changchun 130024, Jilin, People's Republic of China

E-mail: hlxu@nenu.edu.cn, zmsu@nenu.edu.cn

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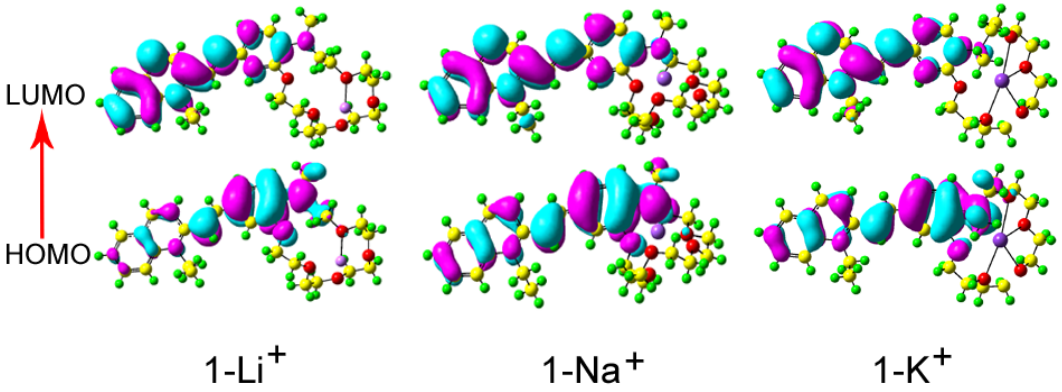
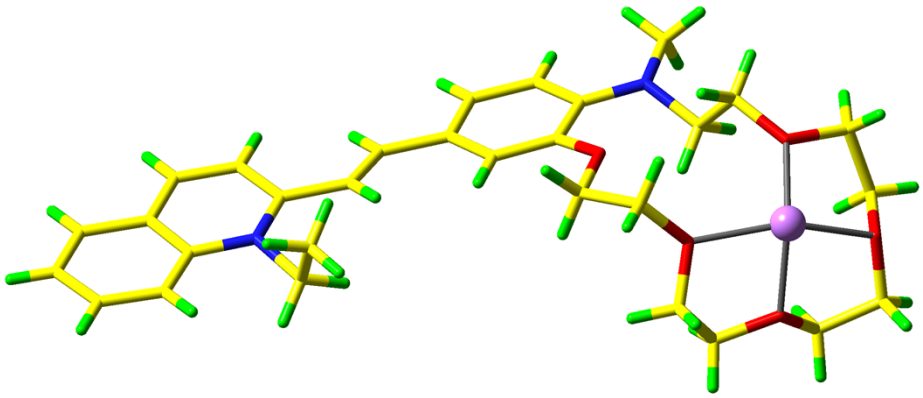


Figure S1 Frontier orbital of **1-Li**$^{+}$, **1-Na**$^{+}$ and **1-K**$^{+}$ with BHandHLYP method.

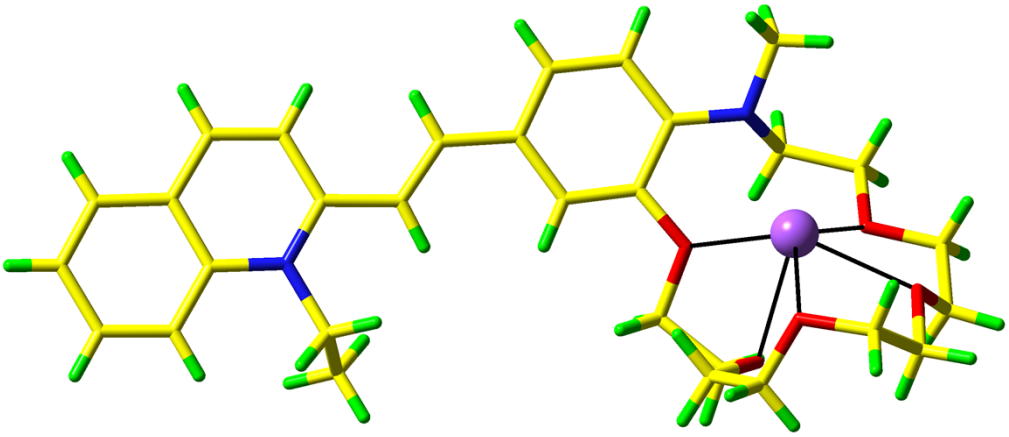


1-Li^{+} **Energy** = -1658.0653 au

Atom	Coordinates		
	X	Y	Z
Li	5.70070000	6.23840000	3.64720000
O	4.47360000	2.68610000	5.61530000
O	5.49690000	5.38390000	5.56970000
O	7.55950000	6.46630000	4.38380000
O	6.80990000	6.67990000	1.87180000
O	4.85910000	4.87610000	2.46300000
N	4.82330000	-0.92750000	11.97730000
N	4.67700000	1.22790000	3.30090000
C	4.70510000	-1.55350000	10.79980000
C	4.59920000	-2.95870000	10.79300000
H	4.55000000	-3.41850000	9.96360000
C	4.57820000	-3.66230000	11.94520000
H	4.50710000	-4.60950000	11.92660000
C	4.65930000	-2.98070000	13.16990000
C	4.59630000	-3.70390000	14.42170000
H	4.52200000	-4.65180000	14.41660000
C	4.64680000	-3.03810000	15.60420000
H	4.60800000	-3.51330000	16.42690000
C	4.75410000	-1.63480000	15.59580000
H	4.78880000	-1.16740000	16.42180000
C	4.81880000	-0.92190000	14.42000000
H	4.87440000	0.02530000	14.43860000
C	4.79960000	-1.59610000	13.21050000
C	4.68580000	-0.78990000	9.55820000
H	4.58360000	0.15190000	9.61220000
C	4.80410000	-1.34110000	8.35870000
H	4.89640000	-2.28750000	8.33510000
C	4.81670000	-0.64720000	7.06130000

C	4.72690000	0.73170000	6.97520000
H	4.70870000	1.25330000	7.76750000
C	4.66940000	1.35240000	5.74370000
C	4.73170000	0.62110000	4.55100000
C	4.81860000	-0.75110000	4.66590000
H	4.85950000	-1.27270000	3.87360000
C	4.85740000	-1.40760000	5.90250000
H	4.90450000	-2.35460000	5.94640000
C	4.43960000	3.51830000	6.78940000
H	5.26950000	3.40180000	7.31810000
H	3.66680000	3.28080000	7.35870000
C	4.32150000	4.95160000	6.30450000
H	3.52500000	5.03050000	5.72000000
H	4.18670000	5.54810000	7.08330000
C	6.52620000	5.86080000	6.39740000
H	6.57980000	5.31540000	7.22180000
H	6.35130000	6.80070000	6.65420000
C	7.80930000	5.76870000	5.64230000
H	8.54580000	6.20490000	6.14400000
H	8.05570000	4.82450000	5.47680000
C	8.56170000	6.25700000	3.41750000
H	8.64920000	5.29040000	3.22490000
H	9.43000000	6.59190000	3.75030000
C	8.16840000	6.98800000	2.18770000
H	8.26720000	7.96350000	2.33130000
H	8.75680000	6.72300000	1.43760000
C	6.72590000	5.48230000	1.04400000
H	7.27940000	4.74980000	1.42070000
H	7.02310000	5.66550000	0.11830000
C	5.22670000	5.13560000	1.09640000
H	4.69370000	5.88990000	0.74160000
H	5.04490000	4.33690000	0.54060000
C	4.24490000	3.58550000	2.73840000
H	3.69460000	3.31040000	1.96300000
H	3.64590000	3.66740000	3.52390000
C	5.29090000	2.53450000	3.01210000
H	5.88530000	2.45010000	2.22480000
H	5.84330000	2.81430000	3.78410000
C	4.62180000	0.36600000	2.12010000
H	4.19570000	-0.48510000	2.35830000
H	5.52850000	0.19820000	1.79240000
H	4.09610000	0.80700000	1.41900000
C	5.11660000	0.58130000	12.01100000
H	5.71800000	0.78740000	12.77120000

H	5.57630000	0.85000000	11.17480000
C	3.87090000	1.32780000	12.15130000
H	4.06680000	2.28840000	12.15630000
H	3.43490000	1.07820000	12.99080000
H	3.28050000	1.11930000	11.39780000

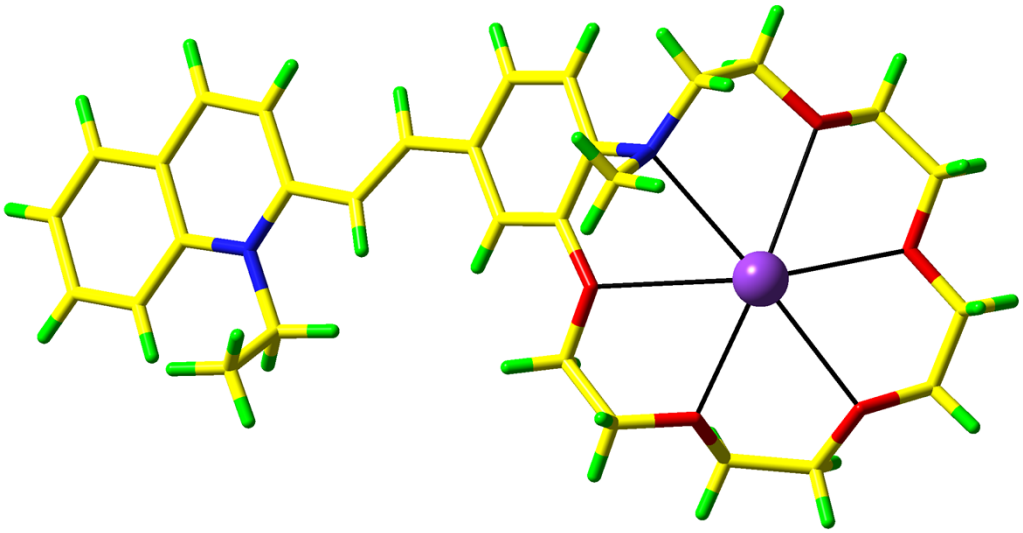


1-Na$^+$ **Energy** = -1812.8258 au

Atom	Coordinates		
	X	Y	Z
Na	0.61950000	4.67780000	2.86440000
O	-0.09790000	5.00790000	5.34190000
O	0.92080000	2.64580000	4.29850000
O	2.77140000	3.30720000	2.37260000
O	0.30060000	2.97410000	1.03310000
O	-1.71740000	4.22260000	2.49710000
N	3.43310000	7.21770000	11.53310000
N	-1.26600000	6.91980000	3.82450000
C	4.10780000	7.64890000	12.69930000
C	4.78470000	6.76400000	13.54000000
H	4.78190000	5.83460000	13.34210000
C	5.45670000	7.22140000	14.64670000
H	5.91930000	6.60910000	15.20640000
C	5.46250000	8.60390000	14.95530000
H	5.94720000	8.92050000	15.70870000
C	4.76930000	9.48390000	14.17000000
H	4.76080000	10.40520000	14.39980000
C	4.06270000	9.04730000	13.01860000
C	3.35380000	9.91870000	12.17150000
H	3.33600000	10.84670000	12.37370000
C	2.69460000	9.46890000	11.07340000
H	2.20910000	10.07680000	10.52850000
C	2.73020000	8.07610000	10.73710000
C	1.98560000	7.57220000	9.57720000
H	1.94850000	6.63170000	9.44740000
C	1.35150000	8.35230000	8.68760000
H	1.36810000	9.28560000	8.86630000

C	0.64750000	7.94910000	7.48940000
C	0.07260000	8.93590000	6.67210000
H	0.12920000	9.84720000	6.93390000
C	-0.57290000	8.61120000	5.49520000
H	-0.95830000	9.30480000	4.97380000
C	-0.67590000	7.28230000	5.04820000
C	-0.07250000	6.28860000	5.87610000
C	0.56090000	6.58550000	7.06580000
H	0.93580000	5.89260000	7.59790000
C	-1.54540000	8.04050000	2.91570000
H	-0.75630000	8.61780000	2.85610000
H	-2.30340000	8.55790000	3.26050000
H	-1.76390000	7.69380000	2.02610000
C	0.12950000	3.91720000	6.24430000
H	-0.54970000	3.91560000	6.96580000
H	1.02770000	3.98940000	6.65510000
C	0.02550000	2.65080000	5.41430000
H	0.22230000	1.86990000	5.98890000
H	-0.90310000	2.55790000	5.08230000
C	2.30450000	2.76140000	4.64810000
H	2.52200000	2.15080000	5.39730000
H	2.51370000	3.68820000	4.92480000
C	3.09680000	2.39180000	3.42860000
H	4.06560000	2.43700000	3.62870000
H	2.87900000	1.46600000	3.15200000
C	2.65690000	2.67370000	1.08330000
H	3.38540000	2.01230000	0.97900000
H	2.75730000	3.35590000	0.37460000
C	1.32980000	1.98020000	0.92370000
H	1.28250000	1.53630000	0.03830000
H	1.21650000	1.29300000	1.62600000
C	-1.00460000	2.36360000	1.18120000
H	-1.02530000	1.79220000	1.98990000
H	-1.21020000	1.79930000	0.39370000
C	-2.01480000	3.47760000	1.30250000
H	-1.96540000	4.07000000	0.51080000
H	-2.92970000	3.10200000	1.35570000
C	-2.73420000	5.23090000	2.67520000
H	-3.62400000	4.80060000	2.73480000
H	-2.73830000	5.84350000	1.89840000
C	-2.46090000	6.01240000	3.93730000
H	-3.25880000	6.55710000	4.15860000
H	-2.31420000	5.37740000	4.68430000
C	3.55430000	5.76710000	11.15210000

H	4.41820000	5.41270000	11.47990000
H	3.54230000	5.68380000	10.16670000
C	2.41670000	4.94950000	11.74160000
H	2.51880000	4.01080000	11.47990000
H	1.56080000	5.29040000	11.40750000
H	2.43540000	5.01950000	12.71850000



1-K^{+} **Energy** = -2250.4211 au

Atom	Coordinates		
	X	Y	Z
O	1.74080000	3.39590000	16.78330000
N	-0.80940000	0.26310000	10.46810000
N	3.78510000	2.13340000	17.99910000
C	-1.21580000	-0.33280000	9.26430000
C	-2.14980000	0.28840000	8.40050000
H	-2.50710000	1.13980000	8.62400000
C	-2.54180000	-0.33390000	7.24110000
H	-3.15120000	0.10450000	6.65750000
C	-2.05310000	-1.61520000	6.90400000
H	-2.35460000	-2.04780000	6.11350000
C	-1.14370000	-2.23220000	7.72020000
H	-0.81180000	-3.09140000	7.48830000
C	-0.68730000	-1.59430000	8.91790000
C	0.29970000	-2.19370000	9.75020000
H	0.66360000	-3.04260000	9.52760000
C	0.71830000	-1.53850000	10.86910000
H	1.40290000	-1.92480000	11.40080000
C	0.15970000	-0.29240000	11.26220000
C	0.59530000	0.38910000	12.47470000
H	0.36670000	1.30330000	12.59350000
C	1.31450000	-0.23590000	13.43810000
H	1.49560000	-1.15860000	13.29910000
C	1.84190000	0.35210000	14.66400000
C	2.79170000	-0.36840000	15.39300000
H	3.00290000	-1.25610000	15.13130000

C	3.43270000	0.18930000	16.49280000
H	4.08360000	-0.31840000	16.96350000
C	3.13200000	1.48890000	16.91500000
C	2.07690000	2.17700000	16.24970000
C	1.47040000	1.62920000	15.12470000
H	0.80050000	2.12050000	14.66470000
C	4.59920000	3.30700000	17.56900000
H	5.35380000	2.99910000	17.02500000
H	4.93610000	3.77740000	18.36100000
H	4.04230000	3.91470000	17.04090000
K	1.76320000	3.42240000	19.67430000
C	0.65430000	4.11250000	16.21470000
H	-0.16940000	3.56310000	16.23290000
H	0.85420000	4.35400000	15.27470000
C	0.47440000	5.36430000	17.05680000
H	1.30200000	5.90470000	16.99540000
H	-0.26060000	5.90110000	16.66760000
O	0.18840000	5.13620000	18.41790000
C	-1.13730000	5.03230000	18.76160000
H	-1.48970000	4.17580000	18.41110000
H	-1.63800000	5.76410000	18.32230000
C	-1.39600000	5.09150000	20.24790000
H	-2.11200000	4.44270000	20.46180000
H	-1.74210000	5.99450000	20.46410000
O	-0.19590000	4.80400000	21.17200000
C	-0.67770000	4.04270000	22.30090000
H	-1.45100000	3.50160000	22.00270000
H	-1.00800000	4.67790000	22.98600000
C	0.28540000	3.15520000	22.92910000
H	1.01990000	3.69630000	23.31370000
H	-0.15680000	2.67330000	23.67110000
O	0.82530000	2.22250000	22.03910000
C	1.63420000	1.22990000	22.59680000
H	1.08710000	0.67510000	23.20900000
H	2.34600000	1.66000000	23.13390000
C	2.25450000	0.36100000	21.59080000
H	2.80070000	-0.33500000	22.03460000
H	1.55350000	-0.08910000	21.05590000
O	3.08000000	1.15280000	20.73950000
C	3.78630000	0.39040000	19.71980000
H	4.38220000	-0.27010000	20.15230000
H	3.13290000	-0.10260000	19.16220000
C	4.55020000	1.25090000	18.90040000
H	5.15910000	0.69670000	18.35190000

H	5.11210000	1.81720000	19.48770000
C	-1.48130000	1.52980000	10.88230000
H	-1.43270000	1.61720000	11.86740000
H	-2.43700000	1.49040000	10.62700000
C	-0.83600000	2.76070000	10.23360000
H	-1.30330000	3.56950000	10.52910000
H	-0.89710000	2.68620000	9.25900000
H	0.10670000	2.81320000	10.49720000